Proceedings of the EYCN Symposium – 1st Edition

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Torino 2018

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European Chemical Sciences
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Dear participants,
welcome to the 1st edition of the **EYCN Symposium**, the scientific event organized by the Italian Chemical Society and the European Young Chemists' Network within the XIII EYCN Delegate Assembly.

This symposium is fully devoted **to young researchers**, such as MSc and PhD students, post-doc fellows and young researchers in companies. All the disciplines of **Chemistry** are covered: analytical, physical, industrial, organic, inorganic, theoretical, pharmaceutical, biological, environmental, macromolecular and electrochemistry.

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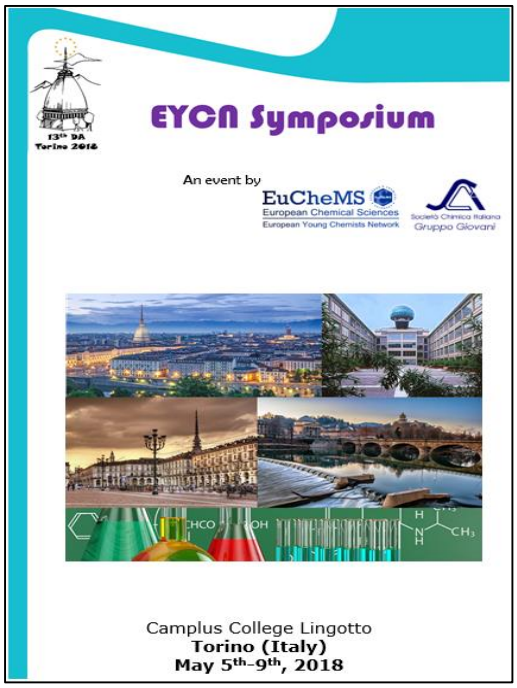

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OR-1

Galloyl-terminated dendrimers modulate Aβ42 fibrillization and reduces cellular toxicity

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Alzheimer's disease (AD) is characterized by the occurrence of extracellular senile plaques of aggregated amyloid-beta peptide (Ab42). These plaques are generated by the self-assembling of Ab42 monomers into supramolecular nanofibrillar structures stabilized by the peptide's β-sheets. While the senile plaques are a hallmark of AD, the presence of intracellular soluble Ab42 oligomers (precursors of the senile plaques) are reported to be the main cause of its toxicity [1].

We have previously demonstrated that the use of natural polyphenols can rescue cell viability affected by the Ab42 fibrillization. In fact, the use of EGCG as a modulator of Ab42 self-assembly has been studied, and its ability to block the assembly process has been reported [2]. The activity of EGCG is reported to occur through the interference of the Pi-Pi stacking within the Ab42 supramolecular arrangement [3]. In general, most of the natural polyphenols reported to modulate Ab42 self-assembly present galloyl-type moieties. Based on this observation, we designed dendrimers displaying this type of moieties on their surface and tested them for their ability to modulate Ab42 fibrillization.

We synthesised a G0-GA core dendrimer with two gallates, and a G1-GA one with six gallate groups. We used CD, DLS and fluorescence spectroscopy to evaluate their ability to inhibit Ab42 fibrillization. Our results show that G1-GA is able to decrease the β-sheet content of the Ab42 supramolecular assemblies, while reducing the size of the fibrils. We also confirmed that G1-GA has the capacity of maintain SH-SY5Y cell viability, reducing the oligomeric Aβ42 assemblies in the cytoplasm of the cells. Our results demonstrate that G1-GA dendrimer represents a promising custom-made nanotherapeutical tool able to modulate the toxicity of Ab42 assemblies in the AD context.

Acknowledgments: Authors acknowledge the fellowship "NORTE-08-5369-FSE-000037". This work was also supported by: H2020-TWINN-2015-692333 (CHEM2NATURE); H2020-WIDESPREAD-2014-2-668983 (FORECAST); GRC2014/040 and Accreditation 2016-2019, ED431G/09 and the European Union (ERDF and H2020).

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[3] A. Attar, F. Rahimi, and G. Bitan, *Trans Neuro*. **4** (2013) 385-409.

OR-2

Supramolecular multilayered biomaterials as instructive platforms to control cell behavior

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Over the last decades, scientists have been inspired by fascinating natural systems to develop supramolecular biomaterials aimed at recreating the complex composition, structure, dynamic and functional behavior of native extracellular matrix (ECM) [1]. Although very promising, most of the developed systems still lack control in thickness, composition, and the functional dynamic nature and structural complexity found in biological systems, which limits many biomedical applications. Herein, we report the successful fabrication of supramolecular multilayered biomaterials comprising marine-origin polysaccharides and oppositely charged self-assembling peptide amphiphiles (PA) by combining the molecular self-assembly strategy with the electrostatic-driven Layer-by-Layer (LbL) assembly technology [2]. Alginate, an anionic biocompatible polysaccharide, was used to trigger the self-assembling capability of positively charged PA molecules. The LbL technology was further employed to fabricate supramolecular multilayered biomaterials with tailored composition, structure and function at the nanoscale, by repeating the alternate deposition of both molecules. The fabrication process was monitored by quartz crystal microbalance with dissipation monitoring. The morphological properties were studied by atomic force microscopy and transmission electron microscopy, revealing the nanofibrous structure of the assembly formed by the two molecules. The *in vitro* biological performance of the supramolecular biomaterials was assessed using C2C12 cells. An enhanced cell behavior was observed on the supramolecular systems having peptide amphiphiles as the outermost layer, showing great promise for being used as supramolecular ECM-like platforms for biomedical applications, including those in muscle and neural tissue regeneration.

Acknowledgments: JB and MPS acknowledge the financial support by the Portuguese Foundation for Science and Technology (FCT) through the Postdoctoral (SFRH/BPD/103604/2014) and PhD (SFRH/BD/97606/2013) grants, respectively. This work was supported by the European Research Council grant agreement ERC-2014-ADG-669858 for project "ATLAS".

[1] M. J. Webber, E.A. Appel, E.W. Meijer, and R. Langer, *Nature Mater.* **15** (2016) 13-26.
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OR-3

Designing polymer electrolytes for sodium-based batteries

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Here, we offer an overview of our recent developments on innovative polymer electrolytes for sodium-ion batteries. Polymer electrolytes were prepared through different techniques, including simple solvent casting [1] and UV-induced photopolymerization (UV-curing) [2,3], being simple, low-cost and easily scalable to an industrial level. All samples were thoroughly characterized in the physico-chemical and electrochemical viewpoint. They exhibited an excellent ionic conductivity of 1 mS cm^{1} at 25 °C and wide as and wide electrochemical stability window (4.7 V vs. Na^{+}/Na), which ensure safe operation at ambient conditions. Electrochemical performances in lab-scale devices were evaluated by means of cyclic voltammetry and galvanostatic charge/discharge cycling using different electrode materials (prepared by water-based procedures exploiting green carboxymethylcellulose as binder).

Work on Na-ion polymer batteries for moderate temperature application is at an early stage, only lab-scale cells were demonstrated so far. Nevertheless, with the appropriate choice and optimization of electrode/electrolyte materials (and successful combination thereof), the intriguing characteristics of the newly developed polymer electrolytes here presented postulates the possibility of their effective implementation in safe, durable and high energy density secondary Na-based solid-state devices conceived for green-grid storage and operating at ambient and/or sub-ambient temperatures.

Acknowledgements: Part of this work is carried out within the activities "Ricerca Sistema Elettrico" funded through contributions to research and development by the Italian Ministry of Economic Development.

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[2] F. Bella, F. Colò, J.R. Nair, and C. Gerbaldi, *ChemSusChem* **8** (2015) 3668-3676.
[3] F. Colò, F. Bella, J.R. Nair, and C. Gerbaldi, *J. Power Sources* **365** (2017) 293-302.

OR-4

Secondary ElectroSpray Ionization (SESI) as a tool for real-time breath analysis

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Exhaled breath contains valuable information about metabolic processes taking place within the human body. Every exhalation contains hundreds of compounds, including metabolites, inhaled exogenous substances and compounds produced in the oral cavity. Since Pauling discovered more than 200 different compounds in exhaled breath using gas chromatography (GC) in the 1970s [1], interest in breath analysis has steadily grown with over 800 compounds identified so far [2].

Interest in studies aimed at identifying clinically relevant exhaled compounds has led to a significant development of appropriate analytical techniques for the detection and identification of human exhaled metabolites. One of such approaches was pointed out by Fenn and co-workers. They noted that gas phase molecules were efficiently ionized in contact with an electrospray cloud at atmospheric pressure, leading to mass spectra akin to that of a sample ionized from the liquid phase. This peculiar way of ionizing vapors has been dubbed "secondary electrospray ionization" or SESI.

Recent studies combining SESI with several commercial high-resolution mass spectrometers (HRMS) have measured limits of detection at sub-ppt levels. This approach is therefore sensitive enough to detect VOCs in minute concentrations in breath, in real time, and can be virtually applied to any commercial MS instrument.

Here we present our contribution to include breath as an alternative body fluid by means of SESI-MS for untargeted metabolomic studies, for non-invasive diagnosis of lung diseases, and for monitoring drugs in exhaled breath.

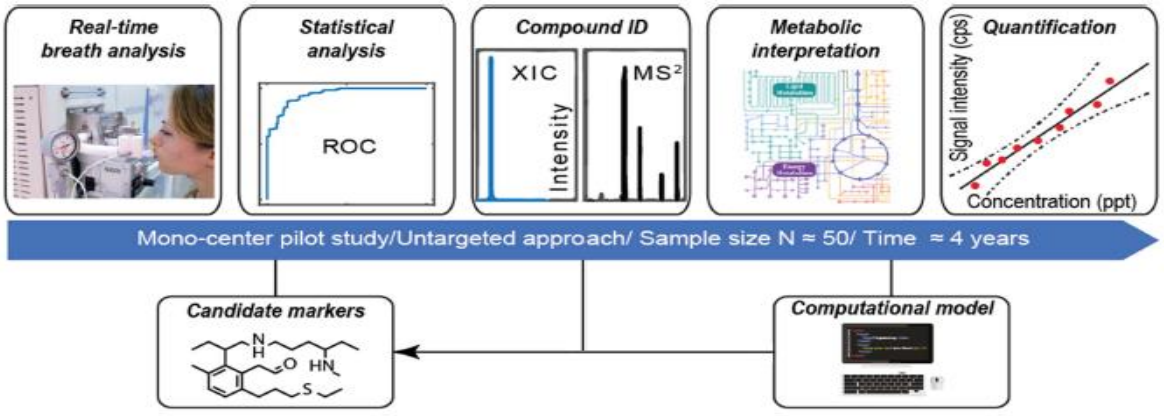

Figure 1: Workflow aiming to the discovery of breath candidate markers.

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OR-5

Enrichment of the epsilon hexachlorocyclohexane isomer in underground water samples

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Almost 50 years after phasing out the production and use of lindane (γ-hexachlorocyclohexane – γ-HCH) in most countries its isomers obtained as side products are persistently causing a global environmental concern. It is estimated that the total amount of HCH isomers is probably around 2-5 million tons, making it probably the most abundant organic pollutant mix in the world [1]. Unfortunately those dump sites are near or within the city limits, such as in Skopje, Macedonia.

Underground water samples around a dump site of HCH isomers were concentrated by liquid-liquid extraction followed by GC–MS analysis. The preliminary results of this investigation gave unusual results: the least abundant ε-HCH isomer from the reaction mixture (2-3 %) at some places is the most dominant HCH isomer in the water samples (as much as ~60 %). This is in line what only one research group has so far reported [2]. Furthermore, 1,3-dichlorobenzene was detected in one of the samples which can be attributed to the degradation of the α-HCH isomer.

We believe that the differences in the amounts can be explained by the microbial environment responsible for a different decomposition rate of the isomers resulting in enrichment of the least degradable isomers.

[1] J. Vijgen, The Legacy of Lindane HCH Isomer Production. A global overview of residue management, formulation and disposal, International HCH & Pesticides Association, 2006, www.ihpa.info/library_access.php (accessed July 2015).
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OR-6

The design, synthesis and evaluation of novel small molecules with potential as anti-diabetic agents

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Diabetes is a chronic condition where suffers display abnormally high blood glucose levels. These high blood glucose levels result from cells inability to take in glucose from the bloodstream. The principle goal of diabetes treatment is to lower blood glucose levels. Complex I is a protein that plays a central role in transforming glucose into energy (ATP). Inhibition of complex I would result in a cell increasing its uptake/supply of glucose from the bloodstream in order to maintain its energy (ATP) levels.

In doing so blood glucose levels would lower [1, 2]. This project aims to develop small organic molecules as inhibitors of complex I, and hence a method for targeting diabetes. The target inhibitors are generated via multistep synthetic pathways and biologically evaluated using a cellular glucose uptake assay.

[1] D.S.D. Martin, S. Leonard, R. Devine, C. Redondo, G.K. Kinsella, C.J. Breen, V. McEneaney, M. F. Rooney, T.S. Munsey, R.K. Porter, A. Sivaprasadarao, J.C. Stephens, and J.B.C. Findlay, *J. Mol. Endocrinol.* **56** (2016) 261–271.
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OR-7

Organic field effect transistors with X-ray photoresponse

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The main problem in characterization of organic compounds is the invasiveness of the X-ray radiation. Many organic materials degrade under the influence of this type of radiation. Some organic semiconductors are very sensitive and even a small dose of the radiation can damage them or cause various changes in their molecular structure and properties [1].

Despite the damage of organic materials, there are also materials which react to electromagnetic waves (not only to visible light but also to X-ray radiation) by generating photocurrent and can be used as sensors or detectors of hazardous radiation doses. Over the past few years some reports about organic X-ray sensors were published, but most devices were based on photodiodes or transistors build from single crystals, nanowires or with the addition of inorganic layers. According to our best knowledge, there are limited scientific reports describing X-Ray sensors based on thin films organic transistors. In one of them OFET based X-ray sensor comprising an additional thin inorganic dielectric layer was constructed [2]. The newest, reports about direct, highly sensitive OFET X-ray sensor [3].

Due to well-known advantages of thin film organic field effect transistors (OFETs) interest on using organic semiconductors as an active layer in X-ray radiation detectors to replace inorganic compounds is constantly growing. This work demonstrates the influence of synchrotron X-ray radiation on thin film OFETs in particular the behavior of the transistor properties like drain current, charge carrier mobilities and threshold voltage. For this purpose as model compounds literature known organic semiconductors were chosen ensuring easy processibility and high charge carrier mobility. These materials were characterized by current-voltage characteristics and grazing-incidence wide angle X-ray scattering (GIWAXS) measurements with and without irradiation.

Acknowledgments: This work is supported by the Foudation for Polish Science in the frame of First team program, First TEAM/2017-3/26.

[1] A. Neuhold, J. Novák, H. G. Flesch, A. Moser, T. Djuric, L. Grodd, S. Grigorian, U. Pietsch, and R. Resel *Nucl. Instrum. Meth. B* **284** (2012) 64-68.
[2] H.N. Raval and V.R. Rao, *IEEE Electr Device L.* **31** (2010) 1482-1484.
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OR-8

A DFT study on the plasma formation of perchlorosilanes

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The amine-induced formation of *neo*-Si_5Cl_{12} from Si_2Cl_6 represents one of the few preparatively efficient synthetic routes to defined perchlorinated oligosilanes known to date [1]. Akin to the relative stabilities of hydrocarbon isomers – and in line with experimental findings – quantum-chemical calculations show that formation of branched silanes is thermodynamically favored over formation of the corresponding *n*-isomers. The plasma-assisted synthesis developed recently in our laboratory provides a unique route to perchlorinated oligosilanes. The latter are formed from $SiCl_4$ and H_2 by $SiCl_4$ polymerization and HCl elimination in a radiofrequency-assisted non-thermal plasma. Surprisingly, the reaction product is composed exclusively of unbranched silanes; plasma synthesis hence provides efficient access to a contra-thermodynamic product.

Here, a detailed quantum-chemical study on the reaction mechanism underlying the plasma-assisted formation of perchlorosilanes is reported. Preliminary results pointed at the involvement of radical cationic species in the reaction course [2]. The initial reaction between H_2 and $SiCl_4^{+\bullet}$ leads to formation of $SiCl_2^{+\bullet}$ as key reactive species that undergoes adduct formation with neutral silanes to yield higher oligosilanes. The proposed reaction mechanism explains the predominant formation of unbranched silanes. Alternative reaction of neutral $SiCl_4$ and H_2 as well as the involvement of other reactive species such as $SiCl_3^+$ are excluded as irrelevant.

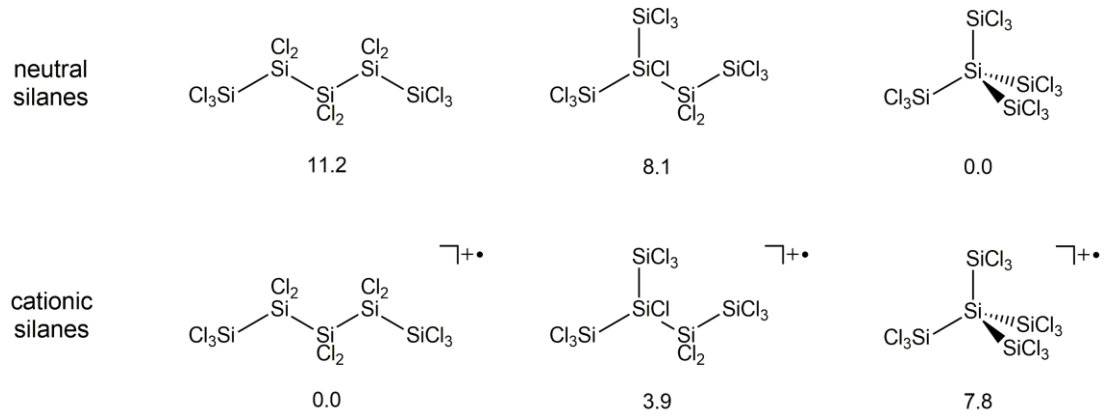

Figure 1: Relative isomer stabilities for neutral Si_5Cl_{12} (top) and radical cationic $Si_5Cl_{12}^{+\bullet}$ (bottom, ΔH^{298} in kcal mol^{-1}).

[1] G. Urry, *Acc. Chem. Res.* **3** (1970) 306-312.
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OR-9

Copper-based heterogeneous catalysts for CO_2 reduction and water oxidation

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Selective electrochemical reduction of CO_2 into energy-dense organic compounds is a promising strategy for using CO_2 as a carbon source. However, efficient and selective earth abundant metal catalysts for the two reactions typically required for efficient CO_2 electrolysis, namely the oxygen evolution reaction (OER) and CO_2 reduction, are still scarce. We will present here the synthesis and electrochemical properties of a rationally designed nanostructured copper/copper oxide electrocatalyst for OER [1], and of a series of Iron-based catalysts synthesized by pyrolysis of iron-, N-, and C-containing precursors for the electroreduction of CO_2 under aqueous conditions [2] (Figure 1). We will present their combination and use in a flow electrolyzer.

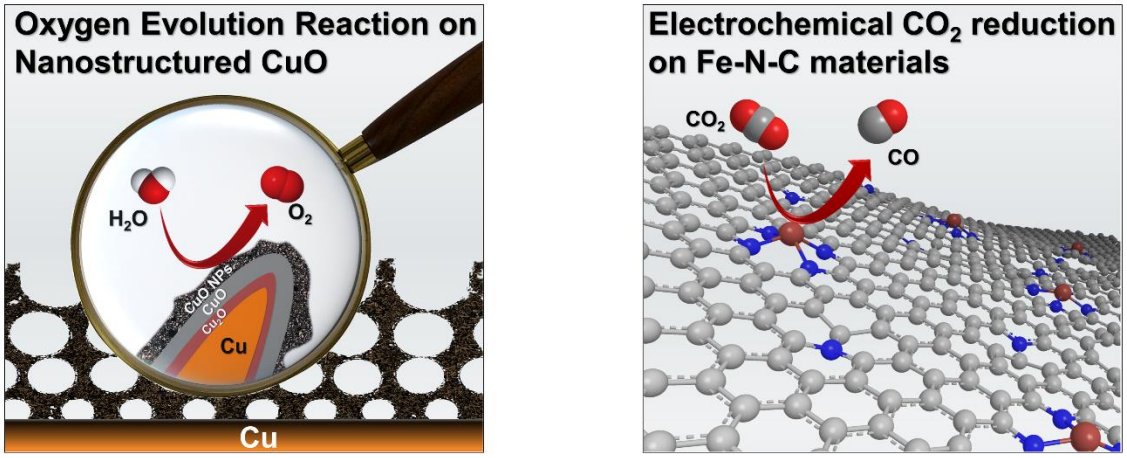

Figure 1: Electrocatalysts for OER and CO_2 reduction (Nanostructured Cu/CuO, left and Cu-N-C material, right).

[1] T.N. Huan, G. Rousse, S. Zanna, I.T. Lucas, X. Xu, N. Menguy, V. Mougel, and M. Fontecave, *Angew. Chem. Int. Ed.* **56** (2017) 4792-4796.
[2] T.N. Huan, N. Ranjbar, G. Rousse, M. Sougrati, A. Zitolo, V. Mougel, F. Jaouen, and M. Fontecave, *ACS Catal.* **7** (2017) 1520-1525.

OR-10

Electrochemical cysteamine assay for the study of reactivity of bioactive ligands

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The detection principle of the assay is based on electrochemical monitoring of cysteamine as model molecule (molecular probe) containing two redox centers, i.e. sulfhydryl and amino groups (Fig. 1A). An amine group can create Schiff bases with various aldehydes, and a sulfhydryl group can be easily oxidized to a disulfide and is a good nucleophile. A typical reaction is Thiol-Michael addition [1,2].

Electrochemical analysis was utilized for observing the interactions of free amino and thiol groups. Therefore, the method could be applied for investigating the reactivity of a broad spectrum of binding ligands to both redox centers of cysteamine. Also, the stability of a battery of thiols and amines under different conditions can be investigated by this method.

Two ligands with well known biological activities and functional groups with different reactivities are involved in the pilot study. Sulforaphane is a natural isothiocyanate (Fig. 1B) and 4-hydroxynonenal is an unsaturated aldehyde produced by lipid peroxidation (Fig. 1C). The reaction products of both ligands with cysteamine were identified using LC-MS.

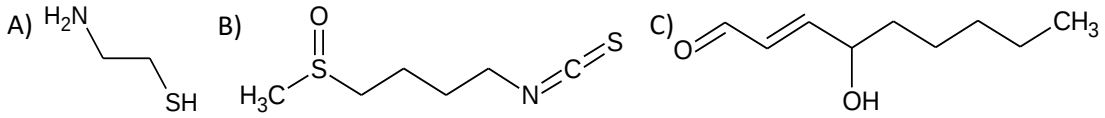

Figure 1: Structures of A) cysteamine, B) sulforaphane, C) 4-hydroxynonenal.

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OR-11

RDC-7119: a crystallographic case study from pharmaceutical development

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RDC-7119 is an *N*-methyl-D-aspartate (NMDA) receptor antagonist and a serotonin reuptake inhibitor discovered at Alkermes. A polymorph screen with 20 solvents and at different temperatures resulted in a single non-solvated polymorph. RDC-7119 crystallized as a freebase with a melt/decomposition temperature starting at 258 °C. RDC-7119 is non-hygroscopic, adsorbing <0.1% mass at 90% RH, and is soluble (0.2 mg/mL) in aqueous media. Single crystals were grown out of acetonitrile and the crystal structure of RDC-7119 showed that it crystallized in the P6(5) space group. A search of the Cambridge Structure Database (CSD) for space group frequency ranking indicated that only 0.07% (272/ 374,246) of CSD entries for organic molecules crystallized in this group [1]. Crystal structure analysis of RDC-7119 showed that one of the hydrogen atoms of the amide nitrogen formed H-bond with the carbonyl of another molecule; and the other hydrogen of the amide is H-bonded with the bridge nitrogen of a third molecule forming a H-bond trimer.

[1] https://www.ccdc.cam.ac.uk/support-and-resources/ccdcresources/a343010d2dfe48f1a577211a2e3e055d.pdf, (499 total in CSD, subtracted by number of inorganic hits from March 31st, 2017 search).

OR-12

Synthesis of novel polyfunctional monomers based on 1,1,3,3-tetramethylguanidine

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Polymer ionic liquids (PILs) are a subclass of polyelectrolytes, which include ionic liquids (ILs) as structural units. According to the type of ion covalently bonded to the polymer chain, PILs are distinguished by anionic, cationic, zwitterionic, and also ionic copolymers. Due to the preservation of the ionized state of the IL units, regardless of the presence of the solvent, PILs are strong polyelectrolytes. Moreover, PILs can be processed using classical methods such extrusion, injection molding, watering, electrospinning, and others. Thus, thin films or fibers can be obtained, which is extremely important for the production of functional materials such as gas separation membranes.

In this work a range of novel polyfunctional monomers based on 1,1,3,3-tetramethylguanidine (TMG) were synthetized and investigated.

Synthesis of new acrylic, methacrylic and vinylaromatic monomers containing 1,1,3,3-tetramethylguanidine fragments was carried out by monoalkylation of TMG by carboxylic acid halides containing unsaturated bonds or p-chloromethylstyrene. The structure of new monomers was proved by using NMR spectroscopy. All synthesized monomers were characterized by a complex of advanced physicochemical methods including Mass Spectroscopy, FTIR spectroscopy and others.

Guanidinium-based compounds demonstrate good performance for the absorption of acidic gasses such as CO_2 and SO_2. Moreover, the guanidinium-based ILs are found to be very useful and efficient in many scientific fields involving catalytic process, dissolution or extraction, and gas absorption.

Acknowledgments: This study was financially supported by Grant of the President of Russian Federation for early stage researchers (MD-4990.2018.3).

OR-13

Cross-linked polymer electrolytes for highly performing lithium batteries working at ambient conditions

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Ion-conducting, self-standing and tack-free poly(ethylene oxide)-based polymer electrolytes are successfully prepared via a rapid and easily up-scalable free radical polymerization, initiated by UV or thermal curing. This procedure is highly advantageous due to its easiness and rapidity in processing, high efficiency and eco-friendliness as the use of solvent is avoided.

The crosslinking produced during curing allows the incorporation of a liquid solvent, RTIL or tetraglyme and LiTFSI salt, leading to a material with remarkable homogeneity and robustness. The cross-linked polymer network can efficiently hold plasticizers without leakage. Samples are thermally stable up to 375 °C under inert conditions. Excellent ionic conductivity (>0.1 mS cm^{-1} at 25 °C), wide electrochemical stability (> 5 V vs. Li), stable interfacial properties and dendrite nucleation/growth resistance are obtained. The lab-scale Li-polymer cells assembled with different electrode materials (e.g., $LiFePO_4$, Li-rich NMC, $LiCoPO_4$, TiO_2) show stable charge/discharge characteristics with limited capacity fading upon very long-term reversible cycling, even at room temperature [1-3].

The overall remarkable performance of the novel polymer electrolytes postulates the possibility of effective implementation in the next generation of safe and durable secondary Li-based polymer batteries working at ambient and/or sub-ambient temperatures.

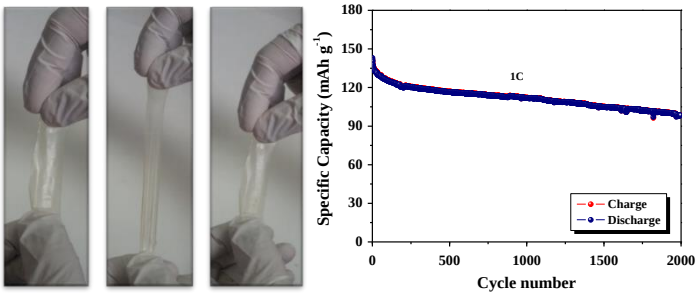

Figure 1. Typical appearance of a cross-linked polymer electrolyte with truly elastic characteristics (left) and long-term reversible cycling at ambient temperature in $LiFePO_4$/Li lab-scale polymer cell (right).

[1] J.R. Nair, L. Porcarelli, F. Bella, and C. Gerbaldi, *ACS Appl. Mater. Interfaces* **7** (2015) 12961-12971.
[2] J.R. Nair, M. Destro, F. Bella, G.B. Appetecchi, and C. Gerbaldi, *J. Power Sources* **306** (2016) 258-267.
[3] L. Porcarelli, C. Gerbaldi, F. Bella, and J.R. Nair, *Sci. Rep.* **6** (2016) art. no. 19892.

OR-14

Nanoindentation of titanium oxide hydrate/polyvinyl alcohol hybrid films after post deposition annealing

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In this work nanomechanical properties of hybrid material of titanium oxide hydrate/polyvinyl alcohol were investigated. These hybrids are perspective for preparation of new types of dielectric mirrors. The reproducibility of the deposition and the homogeneity of the thin films surface are fundamental requirements for the production of highly periodic photonic structures. The main objective was to evaluate the changes produced by post deposition annealing in hybrid thin films. The investigated material was prepared from titanium tetrachloride ($TiCl_4$) and polyvinyl alcohol (PVAl) following a conventional procedure [1].

We investigated a 2.4 μm thick films comprising hybrid with formulation 11.5 mmol titanium per one gram of PVAl, which were deposited via spin coating on glass substrates and aged in vacuum for seven days. Samples were analyzed by Triboindenter (TI750: Hysitron, Minneapolis, USA) using a Berkovich diamond indenter with a tip radius of ~150 nm. Samples before annealing and then annealed 10 minutes at 50 °C, 80 °C, and 200 °C were analyzed.

It was found that roughness slightly increased after annealing. Hardness also increased from 0.26 ± 0.01 GPa for sample before annealing to 1.50 ± 0.04 GPa for sample after annealing 10 minutes at 200 °C. Elastic modulus increased from 3.38 ± 0.09 GPa for sample before annealing to 18.79 ± 0.30 GPa for sample after annealing 10 minutes at 200 °C. Changes in elastic modulus is justified when considering the presence of titanium oxide hydrate units of large dimension that act as point of defect interfering with the polymer-polymer interaction and altering the natural elasticity of the polymer matrix. The annealing promoted the removal of crystallization water and increased the crosslinking density of the hybrid material, hence it justified the observed change of both the elastic modulus and hardness.

Acknowledgments: The work was supported by project VEGA 2/0010/18.

[1] M. Russo, M. Campoy-Quiles, P. Lacharmoise, T.A.M. Ferenczi, M. Garriga, W.R. Caseri, and N. Stingelin, *J. Polym. Sci. Part B Polym. Phys*. **50** (2012) 65-74.

OR-15

First-principles study on the microsolvatation of organic molecules on graphene

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First isolated in 2004 [1], graphene has sparked a great scientific interest thanks to its peculiar mechanical and electronic properties, which promise to upgrade many technologies, from microelectronics to biosensing and nano-medicine [2]. These potential applications require stable graphene dispersions with a good balance between yield and ease of manipulation, where graphene electronic properties are retained. Exfoliation of graphite via non-covalent intercalation of small aromatic molecules represents a promising strategy to obtain high quality graphene while avoiding chemical modifications that can compromise its electronic features.

Among the many molecules that have been proposed as exfoliating agents, only a few successfully exfoliate and stabilize graphene in aqueous media: one example is 2,4,6-triamino-1,3,5-triazine, also known as melamine. In order to explain the role of melamine on stable graphene aqueous dispersions, we have studied the nature of water-melamine-graphene interactions with state-of-the-art density functional theory (DFT) calculations. We analysed different melamine, water and melamine/water coverages and symmetries on graphene within a super-cell slab periodic approach. From our results, we propose a microsolvation model where the subtle interplay between non-covalent interactions, namely dispersion and hydrogen-bonding, provides the necessary thermodynamic driving force to stabilize the graphene-water system with small amounts of melamine [3]. The results discussed in this contribution provide useful insights for the rational design of new non-toxic molecules that can conveniently adsorb with water on graphene, thus enabling its effective use in aqueous media.

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[2] K.S. Novoselov, V.I. Fal'ko, L. Colombo, P.R. Gellert, M.G. Schwab, and K. Kim, *Nature* **490** (2012) 192-200.
[3] A.M. Rodríguez, A.B. Muñoz-García, O. Crescenzi, E. Vázquez, and M. Pavone, *Phys. Chem. Chem. Phys.* **18** (2016) 22203-22209.

OR-16

Imposing unusual reactivity on iridium(III) with redox-active ligands

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The utilization of redox-active ligands has proven successful for tuning the reactivity at a metal center, e.g. by influencing the Lewis acidity and serving as an electron reservoir for catalytic processes.

Based on our previous work [1], we present a series of formally unsaturated Iridium(III) complexes with an unsymmetrically substituted diamidobenzene ligand. Using Meerwein's Salt—a highly electrophilic methylating agent—the Iridium center of compound **1** can be directly methylated, which has recently been shown for Iridium(I) and Rhodium(I) compounds [2,3]. The redox-active nature of the ligands allows reversal of the reactivity at the Iridium center by two-electron oxidation, which opens the Iridium center for nucleophilic attack. The methylated Iridium complex **2** is capable of C-Cl bond activation, which leads to compound **3**.

The complexes and their reactivity have been investigated by various methods including crystallography, cyclic voltammetry, IR-, UV-Vis-NIR- and EPR-spectroelectrochemistry, photometric titration experiments, VT-NMR and mass spectrometry. The electronic structure has been elucidated by (TD-)DFT measurements and Intrinsic Bond Orbitals (IBO).

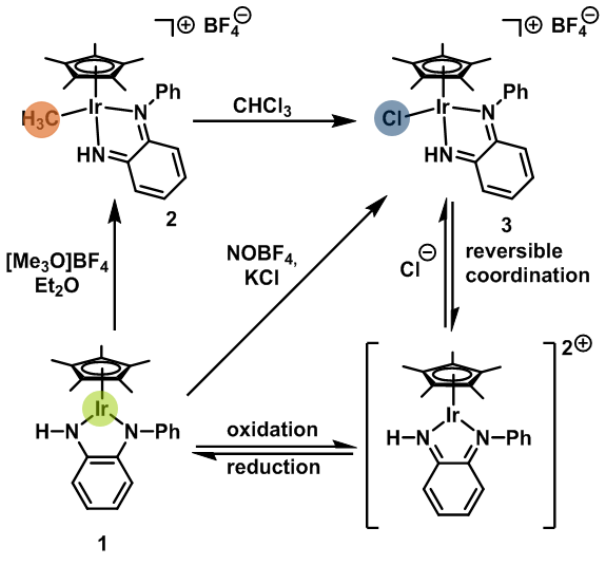

Figure 1: Interconversion of discussed metal complexes.

[1] M. Van der Meer, S. Manck, S. Sobottka, S. Plebst, and B. Sarkar, *Organometallics* **34** (2015) 5393-5400.
[2] C.L. Pitman and A.J.M. Miller, *Organometallics* **36** (2017) 1906-1914.
[3] D. Lionetti, V.W. Day, and J.D. Blakemore, *Organometallics* **36** (2017) 1897-1905.

OR-17

DSSC: a synthetic approach for FRET increasing LHE dyes

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Since the early nineties, dyes have been extensively studied for application in photovoltaic technologies such as dye-sensitized solar cells (DSSC). Large libraries of different kinds of dyes have been synthesized in order to increase solar cell efficiency: natural pigments, ruthenium complexes and metal-free organic compounds are the main categories [1].

Within the last of these families, our group has focused its attention on D-π-A organic molecules. This kind of compounds is characterized by a common motif: an electron rich donor (D) linked to an electron poor acceptor (A) through a highly conjugated spacer. Upon light absorption, this particular structure allows intramolecular charge transfer (ICT) process from donor to acceptor. To have an efficient ICT process molecules must have the HOMO localized over the donor region and the LUMO over the acceptor one [2].

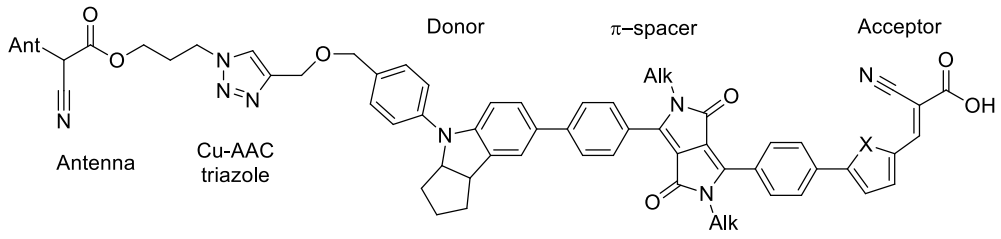

Figure 1: Model of dye-antenna coupled molecule.

Light Harvesting Efficiency (LHE) is one of the critical points for dyes aimed at solar cells application.; on the other hand the design and the synthesis of these compounds, with high molar extinction coefficient in a large range of wavelength, can result challenging.

The aim of this work has been to design a photosensitizer able to exploit Forster Resonance Energy Transfer (FRET) [3] to increase the LHE. This can be realized linking a series of fluorescent donors (antennas) to the dye. These donors must have fluorescence spectra overlapping (<30%) with absorption spectra of dyes and must be spatially adjacent to the chromophore (max 100 Å).

To verify this concept we decided to prepare a model dye to be coupled to a series of fluorescents antennas, using the Cu(I) azido-alkyne coupling (CuAAC) click reaction as a simple and versatile synthetic tool. The methodology is very promising as it might allow the preparation of libraries of dyes to measure the LHE values due to FRET effect.

[1] M.R. Narayan, *Renew. Sust. Energ. Rev*. **12** (2012) 208-215.
[2] Y. Ooyama and Y. Harima, *ChemPhysChem* **13** (2012) 4032-4080.
[3] F. Odobel, Y. Pellegrin, and J. Warnan, *Energy Environ. Sci*. **6** (2013) 2041-2052.

OR-18

Description of explicit solvation by automated water placement based on high enthalpic interactions

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Although many chemical reactions occur in solution, the elucidation of the involved solvated structures still presents a considerable challenge, both experimentally and theoretically.

Quantum chemistry enables us to study the impact of an environment on the electronic structure. While continuum models improve the description compared to simple gas phase calculations, they typically lack the ability to predict structural changes that would occur due to explicit interactions with solvent molecules. Microsolvation, i.e. incorporation of solvent molecules, often improves the description of the effects of the environment on the structure in solution.

When studying microsolvated structures the challenges are where to place the solvent molecules, how many solvent molecules to use and on the other hand which conformations of the solute are relevant in solution. These issues are often attempted to be solved by solely chemical intuition rather than a physics based approach and may not sample the relevant phase space under study.

To resolve these issues, we used a combined Molecular Dynamics and Grid Inhomogeneous Solvation Theory (GIST) [1] approach to analyse the solvent density around the solute. Positions with high enthalpic and entropic interactions with the solute are identified and individual solvent water molecules are placed at these positions to obtain a reliable physically sound microsolvation.

This methodology is applied to various systems ranging from small test systems up to a B_{12} antivitamin, where our results are in line with the solute structure based on NMR spectroscopy.

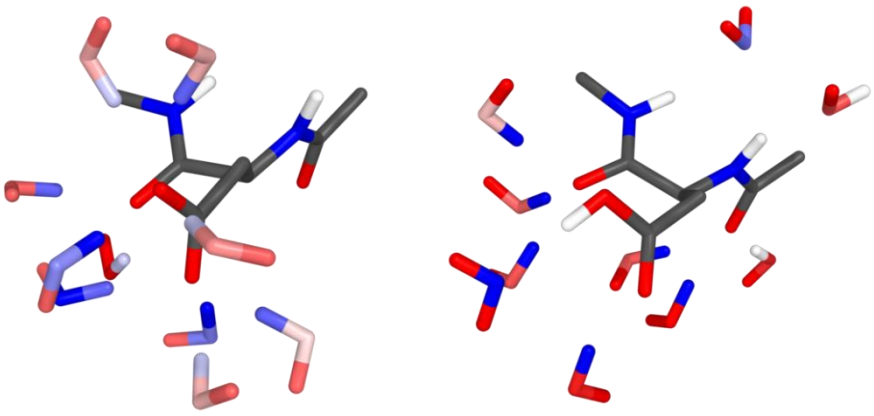

Figure 1: Aspartate deprotonated (left) and protonated (right); atoms of water molecules are color coded according to enthalpic interaction strength (blue strongly, red weakly bound).

[1] C.N. Nguyen, T.K. Young, and M.K. Gilson, *J. Chem. Phys.* **137** (2012) art. no. 149901.

OR-19

The reactions of hypochlorous acid with amino acids

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The reactions of amines, amino acids, peptides and proteins with hypochlorous acid yields *N*-chlorinated compounds under a variety of conditions. In living organisms, these processes are involved in the defence mechanisms against invading pathogens. The very same species are also significant in water treatment technologies where they form spontaneously from dissolved organic species upon dosing chlorine or hypochlorous acid to water. They exhibit disinfecting activity and sufficiently kill microorganisms, though their efficiency is generally less than that of chlorine. In both situations, the biological activities of *N*-chloramines are attributed to their ability of penetrating into the cell where they induce oxidative stress. Ultimately these processes lead to the death of the cells.

In recent years, physiological processes and environmental relevance have generated immense interest in the redox reactions of *N*-chloro-amino acids. Earlier literature results established that the formation of these species from hypochlorous acid and the corresponding amino acids is fast.

Quite frequently, it was assumed that the decomposition proceeds via the Grob fragmentation mechanism and the final products are formed in a single concerted reaction step. Recently, we have shown that the decomposition of *N*-chloroglycine is a far more complex multi-step process. [1]

In this presentation, we report our kinetic results on the formation and decomposition of a great variety of N-chloro-amino acids. The pH profiles of the reactions between hypochlorous acid and amino acids have been explored in detail using stopped-flow technique. The corresponding parameters of activation have been obtained from temperature dependent studies.

N-chloro-amino acids exhibit characteristic spectral bands at around λ_{max} = 255 nm in the UV spectral range, and the decomposition was monitored in this spectral region. Time resolved spectral changes revealed that the decomposition is kinetically coupled with further reaction steps. Kinetic profiles of individual species were also determined and compared by making use of ^{1}H-NMR spectroscopy.

Acknowledgments: This research was supported by the Hungarian Science Foundation (OTKA: K-124983), as well as by the EU and co-financed by the European Regional Development Fund under the project GINOP-2.3.2-15-2016-00008. M. Sz. is indebted to the New National Excellence Program of the Ministry of Human Capacities, Hungary (UNKP-17-3).

[1] M. Szabó, Z. Baranyai, L. Somsák, and I. Fábián, *Chem. Res. Toxicol*. **28** (2015) 1282-1291.

OR-20

How to become a great Teacher

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Everybody can become a great teacher, no matter the "natural born" skills. Just think about the one teacher you had, who left an impact and you know what to do. Knowing your impact as a teacher [1], is knowing what to do. Transferring knowledge is the goal, making the knowledge to last is the challenge. Education in chemistry is one of few disciplines which can combine practice and theoretical in one. One cannot go without the other. So as a teacher or presenter or guest teacher you're blessed with countless ways to teach your audience.

Building your lesson starts with analyzing the audience, exploring their knowledge and how to activate them. Activation is a balance between intrinsic and extrinsic motivation. The starting teacher is mostly focused on the extrinsic motivation, and is slowly moving to the intrinsic motivation using his didactic skills [2]. Having a didactic based teaching plan for a lesson is more than only preparing a PowerPoint presentation, a great teacher chooses learning goals, teaching activities and checks the learning progress matching the goals and uses the feedback from the progress to proceed to the next level [3].

The newest trends are to use digital tools to differentiate within class. Are the used tools really providing the impact wanted? Is a PowerPoint as used presentations supporting the story told or is it a distraction from the story? Being a great teacher is constantly experimenting end evaluating new skills and tools to serve the audience the best way you can.

[1] J. Hattie, *Visible learning for teachers* (2012).
[2] C.A.J. de Jong, W. van den Brink, and J. Leary, *ICL-R Interpersonal Checklist* (2000).
[3] J. Biggs and C. Tang, *Teaching for quality learning at university* (2011).

Società Chimica Italiana

The Italian Chemical Society (Società Chimica Italiana, SCI), founded in 1909 and erected as a Legal Institution with R.D. n. 480/1926, is a scientific association that includes more than 3400 members. SCI members carry out their activities in universities and research institutes, schools, industries, public and private research and control laboratories, or as freelancers. They are joined not only by the interest in chemical sciences, but also by the desire to contribute to the cultural and economic growth of the national community, improving the quality of human life and the protection of the environment.

SCI Giovani / SCI Young

All under-35 SCI members are part of the Young Group. It is an interdisciplinary group that offers several initiatives to its members: the Merck Young Chemists Symposium, the *Primo Levi* and *Reaxys* awards, several workshops like *Y-RICh*, *CV Clinic Day* and *Design Your Future*, useful for the preparation of European projects for young researchers, the creation of collaborative networks, the development of individual soft-skills, and much more.

Please visit our web-site:
https://www.soc.chim.it/it/sci_giovani/home

and follow us in these social networks:

SCI Giovani

SCI Giovani

European Young Chemists' Network

Welcome!

Hello and welcome to the European Young Chemists' Network (EYCN)!

The European Young Chemists' Network (EYCN) is a motivated team of voluntary young scientists from 24 European countries. The EYCN promotes the exchange of knowledge and experience among young chemists in academia and industry, as well as in professional and government bodies across Europe. It provides a platform for the exchange of new ideas and projects, which improves the visibility of chemistry and brings it closer to a wider audience – including partners in industry, business, and management. Moreover, the EYCN supports young chemists at the beginning of their careers with activities focused on soft-skills development for a successful academic or industrial career.

We are glad you want to be part of our team and we are eager to cooperate with you on our journey to connect young chemists all over Europe!

What is the EYCN?

We are a network of 26 chemical societies from **24 European countries** (Figure 1). Each society nominates up to two delegates who will represent them in the annual Delegates Assembly (DA) and in the EYCN throughout the following year.

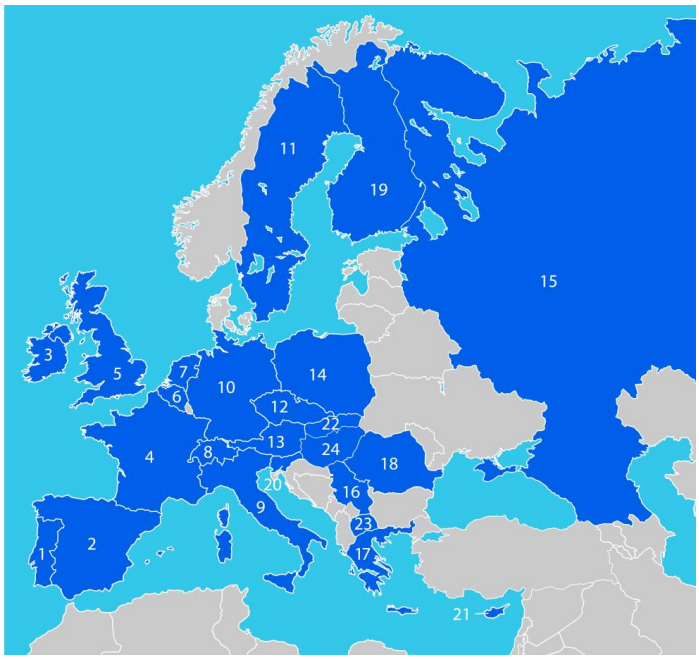
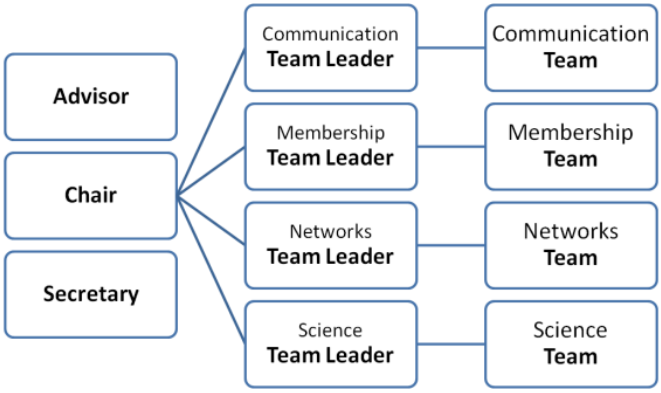


Figure 1. A map of all the countries (showed in blue) which have active delegates in the EYCN: (1) Portugal, (2) Spain, (3) Ireland, (4) France, (5) United Kingdom of Great Britain and Northern Ireland, (6) Belgium, (7) The Netherlands,(8) Switzerland, (9) Italy, (10) Germany, (11) Sweden, (12) Czech Republic, (13) Austria, (14) Poland, (15) Russia, (16) Serbia, (17) Greece, (18) Romania, (19) Finland, (20) Slovenia, (21) Cyprus, (22) Slovakia, (23) Macedonia (FYROM), (24) Hungary.

What are we doing?

The aim of the EYCN is to provide a platform for young researchers in order to connect them and promote chemistry across European countries and beyond.

The EYCN is coordinated by a Board consisting of six members who are elected every two years during the Delegates Assembly (DA) and an Advisor, who is usually the previous Chair. All of the remaining delegates are organized in four teams (Communication, Membership, Networks and Science), which are managed by a Team Leader (Scheme 1).



Scheme 1. The structure of the EYCN Board and Teams.

In the last years, more **than 25 initiatives were coordinated** or supported by the EYCN at a global level, in Europe and abroad. Among these, **19 conferences** were sponsored, and around **20 young chemists were awarded** prizes for their outstanding scientific contributions. Moreover, the EYCN widely advertised and received positive feedback from a large community of chemists for its photography contests '*Photochimica*' and the video contest '*Chemistry Rediscovered'*, aiming at increasing the visibility of chemistry among European high schools. In addition, strong interaction and dynamic action coordination between all EYCN delegates was ensured through the organisation of annual Delegate Assembly meetings and monthly internet meetings.

These events and projects, which simply would not have taken place without the sponsorship of Evonik Industries, have allowed EYCN to publicize the strong support received by Evonik, not only during the events but also through active Social Network advertisement. In Evonik, the EYCN found a great partner and supporter, which trusted on our young network and our activities since our very beginning, and in return has been strongly advertising this very positive support from Evonik to a large number of scientist of broad chemical background.

These events and projects have set strong bases for an ever growing number of new projects, among which the European Young Chemistry Award 2018 (EYCA), the 7th and 8th Young Chemists Crossing Borders (YCCB) exchanges in collaboration with our partners at the American Chemical Society's Younger Chemists' Committee (ACS YCC), the 2nd edition of the '*Chemistry Rediscovered* 'video contest, a Mentoring project for applicants to the Marie Sklodowska Curie Actions and European Research Council grant, but also the co-organisation of the 2nd European Young Chemist Conference or the establishment of a library of soft-skills symposium to be delivered to Young Chemists by EYCN delegates all around Europe. These actions will provide unique opportunities to further advertise and publicize the supports without whom EYCN could not develop.

The following list summarises all of our main activities:

- Public Outreach
    - Publishing articles in newspapers and newsletters
    - Maintaining our website: www.eycn.eu
    - Presence in social media
    - Distributing monthly EYCN newsletters
    - Photo and video contests
- Presence at National and International Events
    - EYCN Career Days
    - Collaboration with COST Actions (European Cooperation in Science & Technology)
    - Organising soft skills Workshops
- EYCN Meetings and Conferences
    - Delegates Assembly (DA)
    - European Young Chemists Meeting
    - EuCheMS General Assembly
- International Exchange
    - Young Chemists Crossing Borders (YCCB) with American Chemical Society
    - Collaboration with IYCN (International Young Chemists' Network)
- Awards and Prizes
    - European Young Chemist Award (EYCA)
    - Poster Prizes at national and international conferences

Detailed overview of EYCN projects:

11th Delegates Assembly in Portugal

- In April 2016, the 11th Delegates' Assembly was held in Guimarães, Portugal. The event had representatives from **16 different European countries** who met to discuss the future plans of the EYCN.

1st Photo contest "Photochimica"

- Under the motto "Chemistry is everywhere!", the EYCN promoted chemistry through visual arts and to showed presence of chemistry in our daily life. The competition was aimed at people under the age of 35 passionate about photography and chemistry. The first edition was a great success: **78 photos from 12 countries** were evaluated and we could organise exhibitions in 5 different countries to display a selection of these photos.

6th EuCheMS Chemistry Conference (ECC) in Seville (Spain)

- During the 6th EuCheMS Chemistry Conference (ECC) in Seville (Spain) in September 2016, the EYCN organized a four-day career event. These "EYCN Career Days" were consisted in lectures and workshops specifically designed by and for young chemists looking ahead to their future career in academia or industry. In order to organise this series of events, the EYCN strongly collaborated with different industries, academic institutions and publishing authorities. This event was jointly organized with the GDCh Career Services & the Careers team of the Royal Society of Chemistry.

Poster award and financial contribution to the Merck Young Chemists Symposium in Italy

- The Merck Young Chemists Symposium is the main international event (**150-200 people**) organized by the Young Group of the Italian Chemical Society, and it is open to the whole EYCN framework. This event promotes the EYCN within Italian young chemists, and this reflects in the strong participation of young Italian scientists to the recent activities promoted by EYCN and EuCheMS.

EYCN meets COST Action CM1407 / NatChemDrug Award

- During the past years, the EYCN established new collaborations with COST Actions, which are a flexible, fast, effective and efficient networking instrument for researchers, engineers and scholars to cooperate and coordinate nationally funded research activities. COST Actions allow European researchers to jointly develop their own ideas in any science and technology field. EYCN promoted an international award for a young chemist in collaboration with the COST Action CM1407. Topic of the call: "Challenging organic syntheses inspired by nature – from natural products chemistry to drug discovery".

1st Video contest "Chemistry Rediscovered"

- This contest promoted chemistry among the young high-school students from all Europe. This was achieved with the help of teachers who developed scientific projects together with their students and encouraged them to present their findings in a form of a video-experiment, together with an accurate experimental protocol. Among **more than 100 videos**, only two per country were selected from a selected national jury to compete at the European level. **15 amazing high-quality videos** and experimental protocols from **8 participant countries** exceeded all expectations for this inaugural edition. After a European evaluation, the winner was announced to be a Portuguese team, which was awarded with a trip to London. Flight and accommodation expenses included, for a 3-night stay, where totally sponsored by Evonik. Places from 2nd to 5th were awarded with participation goodies (participation certificate, T-shirts, calendars, scientific kit). All the videos are currently available on the EYCN Facebook page at: http://www.facebook.com/eycn.eu

Poster Award in Ireland

- The Institute of Chemistry of Ireland hosted a postgraduate conference for all postgraduate chemists in third level institutions in Ireland. This conference included a variety of oral and poster presentations from invited speakers and postgraduate students, from across all fields of chemistry. 2 EYCN poster prizes were awarded during the 69th Irish Postgraduate Colloquium in Dublin.

Treasure Hunt in Greece

- The Treasure Hunt was a project organized by the ReAcTiON team – undergraduate students of Chemistry of AUTH (Aristotle University of Thessaloniki, Greece) in collaboration with the EYCN. The aim was to bring the participants closer to the history and practice of chemistry. Through simple, yet interactive and entertaining procedures and tasks the players were asked to understand chemical terms (e.g. neutralization), solve riddles, and move in space

and time to correct the time discontinuous and be the first to reach the prize. The event hosted **126 participants and 75 volunteers** who were running the game.

12th Delegates Assembly in Greece

- In May 2017, the 12th Delegates' Assembly was held in Heraklion, Greece. The event had representatives from **18 different European countries** who discussed the projects carried out under EYCN flagship during past and future years.

Poster Award in Austria and financial contribution to "Get Together in Austria" event

- As a growing network consisting of 25 working members, the Austrian young chemists have organized their own program at the Austrian Chemistry Days 2017. With workshops, presentations and discussions, the young chemists met before to share ideas between regional teams, made new ones and solved challenges. Furthermore, for the first time in their history, the network has run the first election of the National Board of the Young Chemists Network, who is responsible for the nationwide organisation. Moreover, during the 17th Austrian Chemistry Days, the Austrian Young Chemists Network awarded a poster award for the *very first time*.

Poster Award and the first EYCN Soft-skills Workshop in Serbia

- The Serbian Chemical Society and Serbian Young Chemists' Club organized a mutual event to celebrate the 120th anniversary since the foundation of the Serbian Chemical Society. All Bachelor, Master and PhD students could apply for the 5th Conference of Young Chemists of Serbia. The conference program included poster and oral presentations, as well as soft-skills workshops. One of those was given by the EYCN, where the Chair presented how to design a great poster presentation and to minimize the time-consuming process of preparing and presenting an effective poster.

Oral Presentation Award in Greece

- This project aimed to highlight the importance of high-quality presentations during *the 1st Conference in Chemistry for Graduate*, Postgraduate Students, and PhD candidates in Aristotle University of Thessaloniki, Greece, and to reward the young chemists that gave the best presentations. With this project, EYCN and its activities became better known among the young participants at the conference spreading by this way the vision of the EYCN even further.

Poster award and financial contribution to the Merck Young Chemists Symposium in Italy

- The Merck Young Chemists Symposium is the main international event (**200 young** researchers) organized by the Young Group of the Italian Chemical Society, and it is open to the whole EYCN framework. These occasions let the Italian chemists know about EYCN/EVONIK, and this reflect in the strong participation of young Italian scientists to the recent activities promoted by EYCN/EuCheMS.

Reception JCF in Germany

- The German young chemists' network (JCF) celebrated 20 years and hosted a reception at the Science Forum in Berlin (Wissenschaftsforum Chemie) with

guests from JCF, GDCh, industry and further long-term partners. The event marked a highlight in the anniversary year and aimed to foster future collaboration with existing and new partners. The JCF promoted the "EYCN, partners with Evonik" at this event with advertising of the network to make the EYCN further known in Germany.

Poster Award and financial contribution to the 25th SS PChS in Poland

- The Student Section of the Polish Chemical Society celebrated its 25th anniversary. On this occasion, the board organized a Winter Meeting and promoted the activity of the Student Section and the EYCN among young researchers. The conference program included poster and oral sessions for Bachelor, Master and PhD students coming from all fields of chemistry. Moreover, the board awarded the EYCN poster award for the very first time.

2nd Photo contest "Photochimica"

- In honour to the 150th birthday anniversary of Maria Skłodowska-Curie, the theme of the 2nd edition of Photochimica was 'Radioactivity'. We received around 40 photos from **11 different countries**, such as Austria, France, Georgia, Greece, Italy, Ireland, Netherlands, Poland, Serbia, UK and **the USA**, see Figure 2.
- The 1st exhibition took place in Warsaw during "Medicina-Scientia-Cultura", an International Conference devoted to the achievements of Maria Skłodowska-Curie, which hosted the birthday gala - 150th birthday of the Nobel Prize winner, with the participation of grand-children of Maria Skłodowska-Curie: Hélène Langevin-Joliot and Pierre Joliot. The 2nd exhibition is planned to take place at the 7th EuCheMS Chemistry Congress (ECC7) in Liverpool (UK) from 26th to 30th September 2018.

Figure 2. The winner of the 2nd edition of Photochimica. Title: "12.3" by Thomas Binns (USA).

Contribution to the CrocusExpo, in Russia

- During the International chemical expo "Chemistry-2017" (CrocusExpo, Moscow, Russia), the **first meeting of Young Chemists** was organised in Russia to

establish the Younger Division of Mendeleev Russian Chemical Society (MRCS). During this meeting, the mission and structure of the division were discussed. Around 50 people participated in this first Assembly. The EYCN supported the first Young Chemists Assembly and the formation of the Young Chemists Division and participated with the 2nd Soft-skills Workshop.

Active participation at ABCChem

- Besides European borders, the EYCN actively participated to the inaugural Atlantic Basin Conference on Chemistry (ABCChem) in Cancún (Mexico, January 2018), co-organized by the Chemical societies across North and South America, Europe, and Africa: by the presence of Victor Mougel, the EYCN Networks Team leader and the remote "through internet" interaction of Alice Soldà, the EYCN chair, the EYCN co-organized with the ACS YCC a Young Chemist symposium entitled "a crash course in professional development for young chemists" This event offered a great opportunity for top scientists from around the Atlantic Basin region to share ideas and collaborate on current multi-disciplinary chemistry topics, and for young chemists' networks to establish bridges all around the Atlantic basin.

Presentation Award in Spain

- For the first time, the EYCN was invited to participate to the Trobada De Joves Investigators dels Paisos Catalans in Barcelona for presenting its activities and to sponsor one poster award. The event, organized by the Societat Catalana de Quìmica (SCQ), hosted more than 60 oral presentations given by young researchers and the EYCN contributed with a presentation award.

Presentation Awards in Belgium

- The Chemistry Conference for Young Scientists (ChemCYS) is a biennial scientific meeting for young researchers in the field of chemistry and life sciences. As of 2010, this conference has received an increasing international interest and a growing number of participants, of around **350-400 young chemists**. Due to its international character, the last two editions of ChemCYS were officially endorsed by the International Union of Pure and Applied Chemistry (IUPAC) and the European Association for Chemical and Molecular Sciences (EuCheMS). ChemCYS is organised by the youth division of the Royal Flemish Chemical Society (KVCV), a professional organisation uniting all chemists in Flanders. The Chair of the EYCN was invited to take part at the event as Jury Member and the EYCN contributed to award six students for their excellent poster contributions.

Presentation Award in Portugal

- The Young Chemists Group (GQJ) of the Portuguese Chemical Society (SPQ) is organizing the 6th Portuguese Young Chemists Meeting (6th PYCheM) that will take place in May 2018. Following the success of its previous occurrence, which gathered **more than 200 young** chemists, the 6th PYCheM aims at bringing together young chemists from all over Europe associated with both academia and industry, foster fruitful collaborations, strengthen current scientific and professional collaborations, as well as expand their research network to build up an enlarged international professional network. The EYCN will sponsor a poster award to a young researcher.

Poster Awards in Germany

- The spring symposium of the German young chemists (Frühjahrssymposium des Jungchemikerforums) is an international scientific conference for young chemists. It takes place every year in a different city and is organized by one of the 54 local sections of the Jungchemikerforum. This year, the organizers expect **350 participants from all over Europe**. Besides six plenary lectures, there will be talks by industry and young professionals. There will be 11 oral presentations and up to 300 posters in two poster sessions. The EYCN will sponsor **3 poster awards**.

Poster Award in France

- The French Chemical Society will hold its national congress in June/July 2018 in Montpelier and Toulouse. For the first time, the congress will be entirely held in English and get an international dimension. The RJ-SCF (Réseau des Jeunes Chimistes de la SCF – young chemist networks of SCF) has been actively involved in the conference organization, including the selection of the keynote and invited speakers and the organization of the scientific outreach program. The support of the EYCN to the congress by a poster prize will strongly reinforce the visibility of both young chemists as active organizers and the importance of the EYCN as a structuring member of the European chemistry community.

2nd Video contest "Chemistry Rediscovered"

- The EYCN already received multiple requests regarding the 2nd edition of the EYCN video contest 'Chemistry Rediscovered'. We are glad to announce that this year, *we will collaborate with the EuCheMS Division of Chemical Education*, and the young chemists from all Europe are challenged to present a depicted element from *the Periodic Table in a creative way*. This theme was especially chosen to celebrate the International Year of the Periodic Table and also the centennial of IUPAC in 2019.

What are our aims?

These numerous projects witness for the important achievements accomplished by the EYCN to promote ideas and projects among young chemists, to participate in the structuration of the young chemists' community at a European level and to broadcast soft-skills that are necessary for a successful career in academic or industrial chemistry. These have fostered a broad number of future actions devoted to *i)* further extend our involvement in public outreach events; *ii)* pursue our presence at national and international chemistry-related events; *iii)* organize EYCN meetings and promote the structuration of the Young chemist Community at a European level; *iv)* provide soft-skills trainings to increase attractive of young European chemists on the job market, *v)* establish international collaborations and exchanges and *vi)* be an active actor of the Young Chemists awards and prizes in Europe.

What can you do?

The EYCN lives and thrives through the outstanding work of its members. To keep the EYCN functioning successfully, as it has been so far, it is vital that everyone actively supports all activities.

There are many levels on which you can participate. The list below suggests some of the numerous things you can do to contribute:

- Actively take part in your Team's work
- Promote the EYCN in your country/society
- Organise local and regional events (please inform the EYCN about them)
- Organise talks and workshops (please inform the EYCN about them)
- Raise funding for events related to chemistry
- Help others to organise events and support them with your experience
- …

Each contribution is most valuable! Whether you have a brand-new idea, or if you are supporting and publicising an on-going project, or you are simply giving good advice based on the past experiences. We are always extremely thankful for the engagement and helping to spread the word.

Thank You!

…for your interest and desire to be a part of the EYCN! We hope you will have an exceptional and productive time on our mutual path, to try to make chemistry transparent and bring it to the significant place where it belongs. You will get to know some extraordinary people and different cultures on that way and you can be sure they will all welcome you with open arms and an open mind.

Figure 3. The EYCN Delegates attending the 12th Delegates Assembly in Heraklion (GR).

Follow us!

Please visit our website www.eycn.eu or contact us using our social media profiles on

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Rules of the European Young Chemists' Network

Preamble

The European Young Chemists' Network (hereafter referred to as "EYCN") is the younger members division of the European Association for Chemical and Molecular Sciences (EuCheMS).

§1 Aims and Tasks

EYCN aims to provide a platform within the EuCheMS framework where young chemists can:

a. Contribute to a united voice in science, education and politics – with specific focus on chemistry and molecular sciences - and have their opinions represented throughout Europe;

b. Network with each other to form a supportive community throughout Europe;

c. Forge new links and strengthen old links to facilitate the discussion of common interests between academics and industrialists;

d. Generate and expand upon new ideas and initiatives in order to contribute to the future of science and the development of a European society;

e. Contribute to improving the popular image of chemistry among the general public, therefore enforcing the public awareness of chemistry as a tool to solve societal problems;

f. Have their needs and opinions brought to the attention of the EuCheMS Executive Board and aim for an equal say in EuCheMS initiatives and programmes.

§2 Membership

EYCN's membership exists on an organisational and on an individual level:

a. Members of EYCN are members of EuCheMS under the age of 35 (defined by the constitution of EuCheMS);

b. Member societies of EYCN are bodies representing young chemists of EuCheMS member societies;

c. Affiliate member societies are societies that work closely with EYCN but that are not a part of the EuCheMS framework;

d. Affiliate members are members of affiliate member societies;

e. Delegates are individual members representing a member or affiliate member society;

f. Member societies of EYCN which have resigned as EuCheMS member societies will automatically become affiliate member societies of EYCN.

g. EYCN alumni are former members of EYCN's general assembly.

§3 Institutions of EYCN

The structure of EYCN consists of a general assembly (hereafter called Delegate Assembly), a board and a steering committee.

§3.1 Delegate Assembly

The Delegate Assembly fulfils the role of general assembly for EYCN.

a. The Delegate Assembly (DA) is the highest organisational body of EYCN;

b. The DA is open to all members. Every society within EuCheMS will be invited to appoint one or two delegates of EYCN to represent their respective society;

c. The DA will meet at least once a year in an independent EYCN event. The announcement of the Delegate Assembly will be made at least six weeks in advance of the date. It will consist of at least a tentative agenda, date and place of the DA;

d. The voting body of the DA consists of a single official representative for each of the member societies of EYCN. A delegate may only cast one vote. Each member society may choose to be represented by another delegate through written authorisation. The authorisation must be written and delivered at least 24 hours to the DA and addressed to the Chair of EYCN. For a vote to be valid there is a quorum of 40% of the member societies of the EYCN. The vote will be decided by majority. In the case of a rule change, the quorum will be raised to two thirds of the member societies.

The Delegate Assembly has the mandate to:

a. Decide on the acceptance of new member or affiliate member societies by a majority vote of the delegates during the DA, at which time the new member may be granted voting rights;

b. Evaluate the annual report and decide on the general strategy of EYCN;

c. Decide by majority voting on the need to instate the different board functions (§3.2), number and responsibilities of teams (§3.3);

d. Elect the steering committee by secret ballot. A diverse and equal representation of the different member societies is strived for. No member society may be represented by more than two delegates in the steering committee (§3.4). Voting is done by simple majority. Upon staking of the votes, a single revote is cast. If a single revote offers no solution, decision is made by fate; e.g. by coin toss;

e. Change the "Rules of the European Young Chemists' Network" by a 2/3 majority vote.

§3.2 The board

a. The board of EYCN consists of a minimum of four (4) and maximum of eight (8) members: Chair, Vice-Chair, Secretary and Treasurer and up to four (4) team leaders. The DA may decide not to instate each of these functions if judged unneeded and may choose to have two or more roles fulfilled by the same person. Chair, Vice-Chair, Secretary and Treasurer are defined as in the EuCheMS regulations. Team leaders are defined in §3.3.

b. Members of the board are directly elected by the DA and serve for two years. Voluntary resignation of a board member is possible by sending a written demission with a notice of six (6) weeks, to the Secretary. Upon resignation of a member, responsibilities are taken over by other board members:

    a. Vice-Chair replaces the Chair
    b. Secretary or Treasurer replaces the Vice-Chair
    c. Team leaders may take up the role of Secretary or Treasurer on an interim basis but this should be ratified by the DA.

    Board members may be elected for a second, but not for a third, consecutive term. The Chair may only serve a single term, but will be expected to serve as an advisor for the consecutive term, i.e. they are expected to serve for a further two years as an advisor to the SC. The Chair must represent a different country every term.

c. Forced resignation of a board member will proceed after a meeting of a minimum of 40% of the delegates of the member societies. This can occur between the annual DA at an Extraordinary Delegates Assembly, online if necessary. The vote will be decided by a simple majority.

d. The board directly advises the DA and is responsible for the network's management and the execution of the general strategy of EYCN.

e. The board prepares the annual report and the agenda for the next DA.

f. The board may consult the DA electronically for input and advice, including a request for voting, if circumstances require.

g. The board votes by simple majority. Upon staking of the votes, the Chair decides.

§3.3 Teams

The DA has the right to instate topical teams with well-specified responsibilities.

a. These teams are instated for 2 years and may be reinstated indefinitely;

b. Each team is headed by a team leader. Team leaders are directly elected by the DA. Team leaders may be elected for a second, but not third term;

c. A team is responsible for the performance and oversight of specific tasks of EYCN as decided upon by the DA;

d. Team leaders, each responsible for a team made up from the delegates, will represent their team on the board and in the steering committee.

§3.4 Steering Committee

a. The Steering Committee (SC) will comprise of the board and advisory members;

b. In the absence of the Chair, another board member will act as chair of the SC (analogous to §3.2.B);

c. Each member of the SC shall represent a national society and the diversity of EYCN shall be reflected in the SC. A diverse representation of the different member societies is strived for but not mandatory;

d. The Steering Committee is authorised to amend the rules to incorporate any changes required by EuCheMS Executive Committee;

e. The SC decides on the team's composition, strategy, annual plan and member composition;

f. The SC votes by simple majority. Upon staking of the votes, the chair decides.

§3.5 EYCN Alumni

Former members of the DA have the option of staying on as a member of the EYCN Alumnus programme: EYCN'D.

The alumni have the option to join one of the EYCN Teams or participate in EYCN events. They may also participate in the annual Delegate Assemblies and in SC meetings in an advisory capacity.

§4 Resources

a. Resources should be sought from industry, societies, organisations, individuals or government bodies;

b. Each Team will be responsible for fundraising for their respective projects and will coordinate with a designated board member regarding contracts, invoices, etc., with sponsors and supporters;

c. Invoices in the name of EYCN are issued by the Chair only after approval from the EuCheMS Treasurer;

d. The board will report the financial situation of EYCN at the Delegate Assembly;

e. All resources raised will be used solely for activities of EYCN in a manner approved by the SC;

EYCN will not retain any assets.

EYCN Recognized Events – 2018

DATE	EVENT	CITY (COUNTRY)
January 23–26, 2018	1st Atlantic Basin Conference on Chemistry (ABCChem)	Cancún (Mexico)
January 26–27, 2018	63rd Berzeliusdagarna	Stockholm (SE)
January 27–29, 2018	16th Swiss Snow Symposium ’18	Saas-Fee (CH)
January 28–February 2, 2018	12th European-Winter School on Physical Organic Chemistry (E-WiSPOC)	Bressanone (IT)
January 29–30, 2018	10th Trobada de Joves Investigadors dels Paisos Catalans	Barcelona (ES)
February 21–23, 2018	14th Chemistry Conference for Young Scientists (ChemCYS)	Blankenberge (BE)
March 21–24, 2018	20th JCF-Frühjahrssymposium (spring symposium)	Konstanz (DE)
April 25–29, 2018	Spring Meeting	Skorzęcin (PO)
May 3–5, 2018	Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE II)	Budapest (HU)
May 6–9, 2018	13th EYCN Delegates’ Assembly (DA)	Torino (IT)
May 15–18, 2018	6th Portuguese Young Chemists Meeting (PYCheM)	Setúbal (PT)
May 15–17, 2018	21st Conference of Young Scientists in Chemistry	Nizhny Novgorod (RU)
June 17–20, 2018	1st National Meeting of the Swedish Chemical Society	Lund (SE)
June 21–22, 2018	70th Irish Universities Chemistry Research Colloquium	Belfast (IE)
June 30–July 4, 2018	1st Young chemist symposium	Montpelier and Toulouse (FR)
July 3–8, 2018	5th International ChemCH2018 – Congress on Chemistry for Cultural Heritage	Bucharest (RO)
August 26–30, 2018	7th EuCheMS Chemistry Congress	Liverpool (UK)
August 30–31, 2018	5th RSC Early Career Symposium	Liverpool (UK)
September 9 –12, 2018	70th Congress of the Slovak and Czech Chemical Society	Zlín (CZ)
September 19–23, 2018	25th Congress of Society of Chemists and Technologists of Macedonia	Ohrid (MK)
December 3–5, 2018	6th CHAINS - CHemistry As INovating Science	Veldhoven (NL)

7th EuCheMS Chemistry Congress

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International Younger Chemists Network

Vision: Empowering and supporting young chemists to lead positive change

Mission: To create a unified global network of young chemists

Membership:

- Any chemist under 35 or within 5 non-continuous years from completion of their terminal degree
- Currently spanning 6 continents
- Each country is welcome to have 2 delegates in the IYCN
- Chemical societies cannot be members (e.g. IUPAC)

Find us at:

Current Active IYCN Members

iycnglobal.wixsite.com/iycn

Contact Us

: IYCN@IUPAC.org

: /intlyoungerchemistsnetwork

: /IYCN.global

: @IntlYoungerChem

EYCN 13th DELEGATES ASSEMBLY
PROGRAM

Saturday, 5th May 2018

Time	Program	Moderator
14:00	Check-in at the hotel (for participants that booked sightseeing)	
15:00	Touristic visit to riverside *Guided tour at the Medieval Village and Castle*	SCI Giovani
20:00	Dinner *Italian Tavern*	
22:00	Saturday Night Beer	

Sunday, 6th May 2018

Time	Program	Moderator
9:30	Breakfast	
10:15	Touristic visit to the city centre	SCI Giovani
11:40	Short brunch	
12:20	Touristic visit to Turin heart *Guided tour at Mole Antonelliana* *Guided tour at Cinema Museum*	SCI Giovani
14:00	Check-in at the hotel (for participants that did not book sightseeing)	
15:00	Welcome by Local Committee of Gruppo Giovani – Italian Chemical Society (SCI)	Federico
15:20	Delegates' flash presentations of the member societies (max. 5 min for max. 5-10 PPT slides)	Alice
16:30	Ice Cream Time	
17:00	Delegates' flash presentations of the member societies (max. 5 min for max. 5-10 PPT slides)	Alice
18:00	*EYCN Symposium* *Scientific presentations (6 slots x max. 7 min)*	SCI Giovani
18:45	Free time	
19:15	Meet the delegates	Jelena
20:00	Dinner *"Apericena" in the largest square of Europe*	

Monday, 7th May 2018

Time	Program	Moderator
8:15	Breakfast	
9:00	Official Welcome Presentation of the EYCN and activity report EYCN Account and Budget	Alice
9:40	Presentation EYCN Membership Team	Jelena
10:00	Presentation EYCN Science Team	Hanna
10:20	Presentation EYCN Communication Team	Kseniia
10:40	Presentation EYCN Networks Team	Victor
11:00	Coffee Break	
11:30	ACS YCC Presentation (Dr. John Kelly)	Jelena
11:50	ACS YCCB Program Exchange (Jackie O'Neil)	Jelena
12:00	IYCN Presentation (Dr. Maarten van Sisseren)	Victor
12:30	EVONIK Industries Presentation (Matthias Kleff)	Victor
13:00	Lunch *Camplus canteen*	
14:30	14th DA and 2nd EYCheM 2019 Presentation & Discussion	João
15:00	Internal meetings of the EYCN teams	Team Leaders
15:45	*EYCN Symposium* *Scientific presentations (6 slots × max. 7 min)*	SCI Giovani
16:30	Coffee Break	
17:00	EuCheMS Presentation (Prof. Pilar Goya Laza)	Alice
17:30	SCI Presentation (Prof. Angela Agostiano)	Alice
17:45	Professional Association of Chemists – Piemonte & Valle D'Aosta (Dr. Anna Sampò)	Federico
18:00	7th ECC Presentation (Dr. Sarah Thomas - RSC)	Alice
18:30	EYCA Competition (Dr. Federico Bella)	Alice
18:45	EYCN Activities in Liverpool (7th ECC) State of the Art (Dr. Fernando Gomollón Bel)	Alice
19:30	Free time	
20:15	Dinner *Typical Piemontese dinner* *Dress code: quite elegant*	

Tuesday, 8th May 2018

Time	Program	Moderator
8:15	Breakfast	
9:00	Executive Board Meeting (*only for EYCN Board members*)	Board
9:30	Chemistry Education (Menno de Waal)	Alice
9:50	EYCN Activities in Liverpool (7th ECC) Team work	Fernando
11:00	Coffee Break with Group Picture	
11:45	EYCN Activities in Liverpool (7th ECC) Presentation of results	Fernando
12:30	EYCN Activities in Liverpool (7th ECC) Plan and next steps	Fernando
13:15	Lunch *Meat lunch at 8-Gallery*	
14:30	Mobility and Mentoring Portal (Dr. Andreas Bücker -FECCIA- and Silke Voigt -ECEG-)	Alice
15:00	EYCN Teams Presentation of the final line-ups, ideas and future projects + teams' pictures	Alice
15:50	Young chemists activities at IUPAC19	Victor
16:00	The *Webpage on Chemistry* (Miguel Steiner)	Victor
16:15	Coffee Break	
16:45	*EYCN Symposium* *Scientific presentations (9 slots × max. 7 min)*	SCI Giovani
18:00	Pros and Deltas DA	Alice
18:30	DA closing remarks	Alice
19:00	Free time	
20:00	Dinner *True pizza of Naples*	
22:00	Last night drink	

Wednesday, 9th May 2018

Time	Program	Moderator
8:30	Breakfast	
9:15	Farewell	

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